ON LATTICE GAS MODELS FOR DISORDERED SYSTEMS

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Abstract

We consider a Lattice Gas model in which the sites interact via infinite-ranged random couplings independently distributed with a Gaussian probability density. This is the Lattice Gas analogue of the well known Sherrington-Kirkpatrick Ising Spin Glass. We present results of replica approach in the Replica Symmetric approximation. Even with zero-mean of the couplings a line of first order liquid-gas transitions occurs. Replica Symmetry Breaking should give up to a glassy transition inside the liquid phase.

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It is well known[1] that Ising Model is equivalent to Lattice Gas, a system defined in terms of occupation variables τ taking values 0 and 1. The Lattice Gas effective Hamiltonian is formally identical to Ising one[1]. A simple change of variables ($\sigma = 2\tau - 1$) maps each of the two Hamiltonians into the other, provided that Ising external field is related to lattice gas chemical potential by $h - J = \frac{1}{2}\mu$, where J is Ising spin-coupling related to lattice gas site-coupling Φ by $J = \frac{1}{4}\Phi$. This reflects into a simple relation between Ising free energy density and Lattice Gas pressure: $p = h - \frac{1}{2}J - f$. The two systems have therefore the same phase diagram and the same critical behaviour (real gases and Ising magnets are in the same universality class).

For random systems[2] this whole argument breaks down because the relation between chemical potential and magnetic field involves the quenched couplings. As we shall see in the following this reflects in new and unexpected features for the phase diagram of the system.

For Neural Networks the inequivalence between spin(± 1) and occupation $(0, 1)$ variables was already been pointed out and analyzed, see for example [3] and references therein.

Recently much effort has been devoted to develop a description of the structural glass transition[4, 5, 6] within the framework of disordered systems. All these models were however based on Ising Spin variables instead of Lattice Gas ones which would be more appropriate for a condensed matter system. For disordered systems the two kind of variables are not equivalent. To have a comparison term it would be useful to analyze the properties of a mean field disordered lattice gas model.

We consider a system of N sites, an occupation variable τ_k is defined in each site k, τ_k can take the values 0 or 1. The Hamiltonian of the system is taken to be formally identical to the SK's one[8, 9]. The interaction energy between two different (k and l) occupied sites is taken to be ϕ_{kl} and the system is coupled to some external source g. The total effective Hamiltonian is therefore:

$$H_\phi[\tau] = -g \sum_{k=1}^{N} \tau_k - \frac{1}{2} \sum_{l \neq k} \phi_{kl} \tau_k \tau_l \ . \tag{1}$$

In magnetic language g would be the external field, while for a Lattice Gas g is the sum of the chemical potential, the kinetic contribution, and eventually an external force term. The infinite-ranged interaction energies $\{\phi_{kl}\}$ are taken to be quenched independent Gaussian variables with zero mean and

variance Φ/N. In the following we shall take Φ as our unit of energy and set $\Phi \equiv 1$. We also set the Boltzmann constant equal to 1, as a consequence $H,\ f,\ T,\ g$ and ϕ are all dimensionless. Each ϕ_{kl} is taken to be equally distributed and therefore each site interacts with each other.

For a given realization of the ϕ's the partition function is:

$$Z_\phi(\beta; g) = \sum_{\{\tau\}} e^{-\beta H \phi[\tau]} \ . \tag{2}$$

We are interested, as usual when dealing with quenched disorder, to evaluate the averaged free energy density:

$$f(\beta; g) = -\frac{1}{\beta N} \int P[\phi] \ln Z_\phi d\phi \ , \tag{3}$$

this will be done in the following using the replica approach[2, 7, 8].

We have to calculate the averaged n-th power of the partition function:

$$Z_n = \overline{(Z_\phi)^n} = \int (Z_\phi)^n P[\phi] d\phi \ . \tag{4}$$

For integer n we get, after performing Gaussian integration:

$$Z_n = \sum_{\{\tau\}} \exp \left[\sum_k \beta g \sum_a \tau_k^a + \frac{\beta^2}{2N} \sum_{k<l} \left(\sum_a \tau_l^a \tau_k^a \right)^2 \right] \ ,$$

we can reorder the exponent and obtain:

$$Z_n = \sum_{\{\tau\}} \exp \left[\beta \sum_k \left(g \sum_a \tau_k^a - \frac{\beta}{4N} \sum_{a,b} \tau_k^a \tau_k^b \right) \right] \prod_{a,b} \exp \left[\frac{4}{N\beta^2} \left(\frac{\beta^2}{4} \sum_k \tau_k^a \tau_k^b \right)^2 \right] \ . \tag{5}$$

Using Gaussian identities we rewrite (5) as:

$$Z_n = \sum_{\{\tau\}} \exp \left[\beta \sum_k \left(g \sum_a \tau_k^a - \frac{\beta}{4N} \sum_{a,b} \tau_k^a \tau_k^b \right) \right] \times$$

$$\times \prod_{a,b} \int \left(\frac{N\beta^2}{4\pi} \right)^{\frac{1}{2}} \exp \left(-\frac{N}{4} \beta^2 Q_{ab}^2 + \frac{1}{2} \beta^2 \sum_k Q_{ab} \tau_k^a \tau_k^b \right) dQ_{ab} \ , \tag{6}$$

reordering the exponentials and defining:

$$H_Q[\tau] = -\frac{1}{2}\beta^2 \sum_{a,b} \left(Q_{a,b} - \frac{1}{2N} \right) \tau^a \tau^b - \beta g \sum_a \tau^a \ , \tag{7}$$

$$A[Q] = \frac{\beta^2}{4} \sum_{a,b} Q_{ab}^2 \ - \ln \left[\sum_{\{\tau\}} e^{-H_Q[\tau]} \right] \ , \tag{8}$$

we finally get:

$$Z_n(\beta; g) = \left(\frac{N\beta^2}{4\pi} \right)^{\frac{n^2}{2}} \int e^{-NA[Q]} \ d^{n^2}Q \ . \tag{9}$$

The averaged free energy density is given by:

$$f(\beta; g) = \lim_{N\to\infty} \lim_{n\to 0} -\frac{1}{\beta n N} \ln Z_n(\beta; g) \ . \tag{10}$$

In the thermodynamic limit the integral can be estimated by maximizing the integrand, this yields:

$$f_n(\beta; g) = \lim_{N\to\infty} -\frac{1}{\beta n N} \ln Z_n(\beta; g) = \frac{1}{\beta n} \inf_Q \{A[Q]\} \ . \tag{11}$$

The extremum is determined from the saddle point equation:

$$\frac{\partial A}{\partial Q_{ab}} = \frac{\beta^2}{2} Q_{ab} - \frac{\beta^2}{2} \frac{\sum_\tau \tau^a \tau^b e^{-H_Q[\tau]}}{\sum_\tau e^{-H_Q[\tau]}} = 0 \ , \tag{12}$$

that may be rewritten as $Q_{ab} = \langle \tau^a \tau^b \rangle_Q$.

As a first stage we consider saddle points that are symmetric under the Replica Group[2]. Setting $Q_{ab} = q + b\delta_{ab}$ we can write $\sum_{ab} Q_{ab} \tau^a \tau^b = q \left(\sum_a \tau^a \right)^2 + b \sum_a \tau_a$ and $\sum_{ab} Q_{ab}^2 = n(q+b)^2 + n(n-1)q^2$, substitution in (8) and extraction of the $n \to 0$ limit then yields:

$$f = \frac{1}{4}\beta b(2q+b) - (2\pi\beta^2)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \ln \left[1 + e^{\beta(\alpha + z\sqrt{q})} \right] e^{-\frac{1}{2}z^2} \ dz \ . \tag{13}$$

In equation (13) we set $\alpha = g + \frac{1}{2}\beta b$, and the matrix elements satisfy the coupled equations:

$$\rho \equiv q + b = (2\pi)^{-\frac{1}{2}} \int \left[1 + e^{\beta(\alpha + z\sqrt{q})} \right]^{-1} e^{-\frac{1}{2}z^2} \ dz$$

$$q = (2\pi)^{-\frac{1}{2}} \int \left[1 + e^{\beta(\alpha + z\sqrt{q})}\right]^{-2} e^{-\frac{1}{2}z^2}\, dz \ . \tag{14}$$

As can be seen following the line of [8, 9] the physical significance of ρ and q is:

$$\rho = \overline{\langle \tau \rangle} \qquad\qquad q = \overline{\langle \tau \rangle^2} \ , \tag{15}$$

where, following the notations of [2], a bar denotes the average over quenched disorder.

For $\beta = 0$ we have $\rho = \frac{1}{2}$ and $q = \frac{1}{4}$, as we expect from their physical significance. In the high temperature regime we can solve (14) by expansion in powers of β, this yields:

$$\rho = \frac{1}{2} + \frac{1}{4}\beta g + \frac{1}{32}\beta^2$$

$$q = \frac{1}{4} + \frac{1}{4}\beta g + \frac{1}{16}\left(\frac{3}{4} + g^2\right)\beta^2 \ .$$

We have numerically solved equations (14) for several values of T and g. We find a line of first-order phase transitions. Such line ends in a second-order transition point, for $T \simeq 0.22$ and $g \simeq -0.7$, where the linear response function $\chi = \partial\rho/\partial g$ (the "susceptibility") is found to be divergent.

Let us define

$$\gamma_0 \equiv \lim_{T\to 0} \beta(\rho - q) = \lim_{T\to 0} \beta b \ \ ,$$

for $T \to 0$ we have $\rho = q + \gamma T$ and thus $\alpha = g + \frac{1}{2}\gamma_0$. For $\beta \gg 1$ the solution of (14) can behave in two different ways depending on which side of the first order transition we consider. We call $g_0 = -0.63633$ the transition point at zero temperature. In the range $g < g_0$, q_0 $(\equiv q(T;g)|_{T=0})$ and $\gamma_0(g)$ are identically zero (details will be presented elsewhere[11]), we find that all their temperature derivatives vanish for $T \to 0$, q vanishes as $e^{\beta g}$ $(g < 0)$ and γ $(\equiv \beta(\rho - q))$ as $\beta e^{\beta g}$. Elsewhere if $g > g_0$, they depend linearly on T, indeed we get:

$$q = q_0 - \frac{q_0\gamma_0(q_0 + \frac{1}{2}\gamma_0\alpha_0)}{(q_0 + \frac{1}{2}\gamma_0\alpha_0)^2 + \frac{1}{4}\gamma_0(q_0 - \alpha_0^2)}\ T$$

$$\gamma = \gamma_0 + \frac{\frac{1}{2}\gamma_0^2(q_0 - \alpha_0^2)}{(q_0 + \frac{1}{2}\gamma_0\alpha_0)^2 + \frac{1}{4}\gamma_0(q_0 - \alpha_0^2)}\ T$$

$$\rho = q + \gamma T \ .$$

Next we look to thermodynamical functions, the internal energy and entropy densities are given by:

$$u = -(g + \gamma_0)q$$

$$s = -\frac{1}{4}\gamma_0^2 \ . \tag{16}$$

The entropy (16) is negative in the range $g > g_0$ where γ_0 is different from zero, so we should expect the Replica Symmetry to be broken in this region. We stress that differently from SK case we have a region in which the Replica Symmetric Solution remains physical down to zero temperature. This can be related to some exact results on the ground state energy of the model[11]. The maximum absolute value of the zero temperature entropy is at $g = g_0^+$ where it takes the value 0.101 and it strongly decrease for higher values of g (e.g. at $g = 1 \ \ s = -0.011$). This solution is clearly unphysical (for $g > g_0$) at low temperature. This should be considered a clear signal[2] of Replica Symmetry Breaking (RSB).

Now we briefly compare our results with the ones of Sherrington and Kirkpatrick. In SK case the zero-field Hamiltonian has a *global Z_2 symmetry* and all thermodynamical functions are either even or odd in the external field. SK model can have a (field-driven) *first-order phase transition* only if a strong enough ferromagnetic part (i.e. a non-zero mean) is added to the random coupling. Such a transition is indeed related to the breaking of the global Z_2 symmetry induced (as in the homogeneous case) by a ferromagnetic coupling. Moreover, at each value of external field, SK's Replica Symmetric Solution always becomes unphysical for low enough temperature.

It is apparent how our picture is different from the usual one. We have considered the case of purely (zero-mean) random interactions and our Hamiltonian has no Z_2 symmetry. The *Replica Symmetric Solution* of our system exhibits a line of first-order phase transition points ending with a second-order transition. This feature is expected to be robust to *Replica Symmetry Breaking*, as should be confirmed by the stability analysis[10, 11]. Two phases co-exist along the transition line and in one of them the Replica Symmetry should remain *exact down to zero temperature.* Following the conventional Lattice Gas interpretation this two phases should be called 'gas' and 'liquid'.

The gas-like phase is that which is replica-stable at all temperature. When Replica Symmetry Breaking sets up the liquid-like phase can give up to a glassy state. This idea will be put forward elsewhere[11].

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References

[1] K. Huang:
Statistical Mechanics
(John Wiley & Sons, 1963).

[2] M.Mezard, G.Parisi and M.A.Virasoro:
Spin Glass Theory and beyond
(World Scientific (Singapore), 1987).

[3] M.V. Tsodycs and M.V. Feigel'man:
The Enhanced Storage Capacity In Neural Networks with Low Activity Level.
Europhysics Letters **6**(2), 101-105 (1988).

[4] J. P. Bouchaud and M. Mèzard:
Self Induced Quenched Disorder: A Model for the Glass Transition,
J. Physique I **4**, 1109 (1994).
cond-mat/9405075.

[5] E. Marinari, G. Parisi and F. Ritort:
Replica field theory for deterministic models: I. Binary sequences with low autocorrelation,
J.Phys. **A 27**, 7615-7645 (1994).
hep-th/9405148.

[6] E. Marinari, G. Parisi and F. Ritort:
Replica field theory for deterministic models: II. A non-random spin glass with glassy behavior,
J.Phys. **A 27**, 7647-7668 (1994).
cond-mat/9406074.

[7] S. F. Edwards and P.W. Anderson:
Theory of spin glasses
J. Phys. F: Metal Phys., **5**, 965 (1975).

[8] D. Sherrington and S. Kirkpatrick:
Solvable Model of a Spin-Glass
Phys. Rev. Lett. **35**, 1792 (1975).

[9] S. Kirkpatrick and D. Sherrington:
Infinite-ranged models of spin glasses
Phys. Rev. B **17**, 4384 (1978).

[10] J.R.L. De Almeida and D.J. Thouless:
Stability of the Sherrington-Kirkpatrick solution of a spin glass model
J Phys. A **11**, 983 (1978).

[11] Francesco M. Russo:
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